NATIONAL ACADEMY OF SCIENCES
NATIONAL RESEARCH COUNCIL
Washington, D. C. 20418

Commission on International Relations

February 13, 1981

Dr. Meselson:

Our records show the following information regarding visits in the US by V. A. Gubanov, Director, Laboratory of Physical Methods of Solid State Research, Institute of Chemistry, Urals Scientific Center of the Academy of Sciences of the USSR:

Nominated by ASUSSR	7/29/74	6/22/79
Accepted by NAS	11/20/74	10/2/79
Visit began	12/13/74	11/9/79
Visit ended	10/10/75	5/20/80
Duration	10 mo.	6.75 mo.

Lawrence C. Mitchell

JH-222

Staff Director
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DEPARTMENT OF PHYSICS
AND ASTRONOMY

PRIVILEGED

REPORT ON SCIENTIFIC EXCHANGE VISIT OF Donald E. Ellis TO THE SOVIET UNION

Under the auspices of the American National Academy of Sciences/ Soviet Academy of Sciences exchange program my family and I spent the Spring quarter, 1979 in the Soviet Union. Departing from Evanston on April 10, we traveled first to Moscow, where we were met by our host Dr. V.A. Gubanov and a representative of the administration of the Ural Science Center, Mikhael Sveichnikov. After spending two days for rest and orientation, we flew to Sverdlovsk to begin research activities.

Gubanov and I had worked together previously, beginning in 1975, when he came to Northwestern University as an exchangee, and continuing in Sweden during the following year. The collaboration turned out to be quite productive, resulting in several new ideas concerning methods of embedding clusters in solids, and the treatment of relativistic effects. When we arrived in Sverdlovsk, I found that Gubanov had assembled a group of seven very capable young theorists. This group had already succeeded in implementing a version of my molecular cluster program, and also the so-called multiple scattering program, on the local BESM-6 computer. With this tool they were studying the electronic structure of transition metal carbides, nitrides, oxides and related compounds with high melting temperature and great hardness. The experimental program of the Institute of Chemistry (where I was working) and the nearby Institute of Metal Physics strongly influenced the choice of materials for theoretical study. A second theoretical project, concerning the electronic properties of optically active rare-earth compounds was also underway, again stimulated by experimental interest in fluorescence and laser materials.

Several other topics were in early stages of development; these were the areas which Gubanov and I decided required concentrated effort:

1. Description of the magnetic excitation spectrum of insulating and semiconducting compounds, such as NiO and EuO
2. Developing models for the electronic structure and related physical properties of non-stoichiometric compounds, such as NiC_x
3. Extension of embedded-cluster self-consistent models to treat ternary systems like EuOF.
4. Modification of the multiple-scattering technique to include "crystalline boundary conditions" in cluster calculations.
5. Development of perturbative transition state methods for calculating changes in total energy (and hence binding energies) accompanying nuclear motions.

Work on these topics was begun in stages during the first month. In addition, we met with group members several times daily to discuss results of computations and to decide on further steps in applications and in expanding program capabilities. Most discussions were in English, with occasional excursions into Russian. My college-level Russian turned out to be very valuable, and improved slowly, but in the lab most people seemed fairly eager to try their knowledge of English.

We were received everywhere with great kindness and warmth. Of course, the presence of two small boys (ages 1½ and 5) immediately involved us in local family life. The Science Center made available to us a very large apartment, normally used as a kind of guest house for visiting scientists. We adapted rather quickly to the local routine of shopping and house-keeping, under the tutelage of our friends. Help from friends was essential in understanding the very complex system of supply and demand, with various official and unofficial methods of procurement. The living allowance provided by the Soviet Academy proved to be adequate for ordinary needs, with sufficient left over to enjoy the ballet, movies, and an occasional evening at a restaurant.

With a population of 1½ million Sverdlovsk is large enough to have a fairly rich cultural life- although the level of performance naturally enough, doesn't compare with that at Moscow or Leningrad. We traveled freely about the city, and did quite a bit of exploring through the older sections of wooden houses which are gradually giving way to multistorey apartments and office buildings. A number of trips outside the city were made to nearby lakes and villlages. These trips required prior notification to the city authorities, and we were accompanied by friends. We were not aware of any particular restrictions or security precautions- I think some of our Russian friends were a little surprised at the ease with which arrangements were apparently made, since prior to this year Sverdlovsk had been a closed city.

The bureaucracy in Moscow had decided that we should spend one month in Sverdlovsk, followed by two months in Novosibirsk (where supposedly one could mix comfortably with the cream of Siberian scientists in a controlled atmosphere). We had protested this alteration of our plans before leaving the United States, and had been informed that this was negotiable. Once work was underway in Sverdlovsk, it became clear that it was essential to return to our original plan: two months in Sverdlovsk, one month in Novosibirsk. It was quite interesting to observe ensuing developments from the sidelines. My case eventually consumed some time and efforts on the part of Prof. Vonsovsky, who as President of the Science Center and Academician was able to command some attention. Clearly issues of local autonomy were involved. True to stereotype, Moscow gave no clear reply until the last moment, and on May 15 we departed for Novosibirsk, not knowing whether or not we would continue our work begun in Sverdlovsk. It actually took another month to resolve the issue, complete with not-so-subtle hints that we might prefer to return to the States at the end of the second month. Out of this and other experiences, we developed some understanding of the great efforts that are required to achieve any objectives in this system.

We spent one month at the Science Center in Novosibirsk, in the Akademgorodok-scientific suburb of the city. Our host was Prof. L.N. Mazalov of the Institute of Inorganic Chemistry. This institute does not have a strong tradition in theory, but carries out very wide-ranging experimental programs in X-ray and photoelectron spectroscopy as well as the traditional inorganic synthesis and analysis work. An effort was being made to expand the theoretical effort, but the pace was noticeably more relaxed than in Sverdlovsk. The Science Center of the Siberian division of the Academy of Sciences gives an overall impression of being overorganized and complacent- perhaps the results of conscious efforts to build a pleasant

home in a hostile environment. Summertime in Novosibirsk is warm and sunny, with opportunities for boating, picnics, and swimming. People did vividly recall the previous winter with heating restrictions (fuel shortage?) and temperatures below -40°C, so we were grateful to see the "best" time of year.

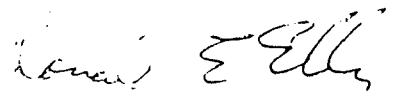
Despite these idyllic diversions, we managed to start up some theoretical work related to the x-ray and photoelectron studies- notably directed toward explaining absorption lineshapes and photoemission cross-sections. We expect that this work, done in association with Anatol Kondratenko, will eventually mature into some kind of collaborative project. The laboratory of Prof. Mazalov has practically unique capabilities for high resolution studies which are required.

The Sverdlovsk projects were meanwhile kept going, as first one and then another member of the group would come to work on particular problems. Since the "new generation" of integrated circuit computers was apparently not working very well, Novosibirsk was also relying on the older BESM-6 machines for scientific computation. One result was a shortage of machine time, and difficulties for foreigners (including Russians from other labs!) to obtain access. The quality and quantity of machine services seems to be a problem- partly connected with the traditional control of computers by the mathematicians. At any rate, it is an obvious impediment to the development of the kind of mathematical modeling which has been so useful in the United States. The minicomputers used to interface experimental equipment seemed to me to be very rudimentary, if used at all.

Toward the middle of June, we learned that our return to Sverdlovsk had indeed been approved. We worked at a busy pace for the remaining time, trying to set the projects I have mentioned into a form which could be completed long-distance. There was time to attend several summer parties, and to verify that my tolerance for vodka had approximately doubled. By departure time rough drafts of several articles had been prepared, and abstracts for meetings both in the USSR, Europe, and the United States prepared.

Discussions with a number of people at the Science Center led to the conclusion that benefits would follow by widening the scope of the Northwestern University-Ural Science Center collaboration, and by adopting some formal recognition of this effort. Certainly from the Russian side, the existence of a "program" would ease the process of obtaining permission and funds for travel. From our own point of view, it should be possible to make more long range plans involving perhaps several people (for example, Prof. Y. Izymov-an expert in magnetism and alloys, already a frequent visitor at Northwestern, and Dr. Ernst Kurmaev-an expert on superconductivity and x-ray emission spectra). I brought back to Evanston a letter from Prof. Vonsovsky, inviting the University to express its interest. Our Dean of Science has responded favorably, so we may expect further developments. Copies of both letters are attached.

A new visit of Dr. Gubanov to Northwestern is in the process of being approved by the National Academy, according to recent information.



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1 Oct. 1979